

4-Butoxybutanoic acid  
55724-73-7 | DTXSID90204272

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 31.6 °C

Global applicability domain: Inside

Local applicability domain index: 5.74e-01

Confidence level: 7.53e-01

Nearest Neighbors from the Training Set

Image not found

9-Cycloheptadecen-1-one

Measured: 32.5

Predicted: 26.0

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Undecanoic acid, 11-fluoro-

Measured: 36.0

Predicted: 30.3

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Decanoic acid, 10-fluoro-

Measured: 49.0

Predicted: 38.1